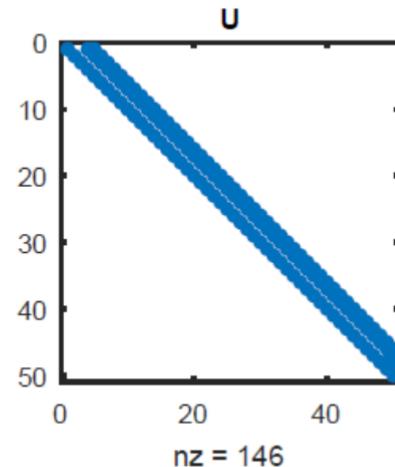
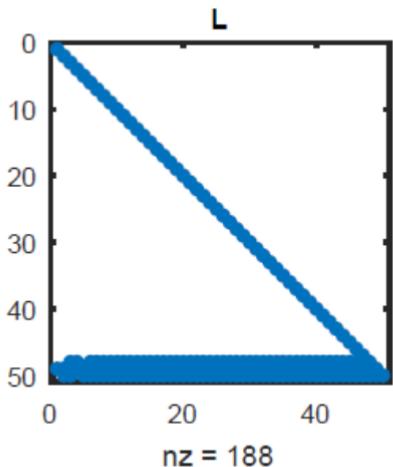


Chapter 8

Krylov Methods in Linear Algebra



Section 8.1

Sparsity and Structure

Methods for large matrices/systems

- We could also have called this chapter “Iterative methods”
- Depending on your computer, you may find it is difficult to store an $n \times n$ matrix where $n = 10^4$ 763 MB
- We need a way to compute at all for larger matrices
- We need ways to compute efficiently for larger matrices

$$n = 10^5 : 74.5 \text{ GB}$$

Sparse matrices

- One common case is when large matrices has many *structural zeros*: many elements are exactly zero
- In these *sparse matrices*, the fraction of nonzero entries may be quite small
- One uses much less storage to store only nonzero entries, and to do computations only for nonzero values
- Each nonzero entry $\{a_{ij}\}$ in the matrix \mathbf{A} can be stored as a triple (i, j, a_{ij})
- One then has to write code that can correctly use only the nonzero entries; we will not do this
- But, we will exploit Matlab's capabilities in this area

Example: large adjacency matrix

Example 8.1.1

A is an adjacency matrix for web pages making about Roswell, NM, and how they link to each other.

```
load roswelladj % get from the book's website  
a = whos('A')
```

```
a =  
    name: 'A'  
    size: [2790 2790] ← • It's large  
    bytes: 158120  
    class: 'double' ← • The elements  
    global: 0  
    sparse: 1 ← • It's sparse!  
    complex: 0 ← • Real valued  
    nesting: [1x1 struct]  
    persistent: 0
```

Example: large adjacency matrix

Example 8.1.1

Each nonzero entry in A corresponds to an edge; we can compute fraction of nonzeros: call that the density

```
sz = size(A); n = sz(1);
density = nnz(A) / prod(sz)
```

size returns the number of rows and columns

nnz returns the number of nonzero elements

Sparse!

full creates the full matrix storage version

Compare storage of sparse vs full matrix versions

```
density =
0.0011
```

```
F = full(A);
f = whos('F');
a.bytes/f.bytes
```

```
ans =
0.0025
```



How about computation time?

Example: large adjacency matrix

Example 8.1.1

Computation time for sparse vs full? Sparse uses only nonzeros

```
x = randn(n,1);
tic, for i = 1:200, A*x; end
sparse_time = toc
```

tic and toc for timing

Matrix vector products first

Create random vector,
repeat 200x for timing

Sparse first, then full

60x slower for full!

```
tic, for i = 1:200, F*x; end
dense_time = toc
```

```
dense_time =
0.6207
```



Example: large adjacency matrix

Example 8.1.1

Computation time for row operations can be slower: Matlab's sparse storage is column oriented

```
v = A(:,1000);  
tic, for i = 1:n, A(:,i)=v; end      Column oriented  
column_time = toc  
  
r = v';  
tic, for i = 1:n, A(i,:)=r; end      Row oriented  
row_time = toc
```

```
column_time =  
    0.0079  
row_time =  
    0.0630
```

8x slower for rows

[Example 8.1.1]

Matrix fill-in

- Arithmetic operations $\ast, +, -, \wedge$ can exploit sparsity
- But, matrix operations can reduce the sparsity: *matrix fill-in*

Example 8.1.2

Here is the buckyball adjacency matrix again.

```
[A, v] = bucky;
```

The number of vertex pairs on a soccer ball connected by a path of length $k > 1$ grows with k , as can be seen here for $k = 3$.

```
subplot(1, 2, 1), spy(A)  
subplot(1, 2, 2), spy(A^3)
```

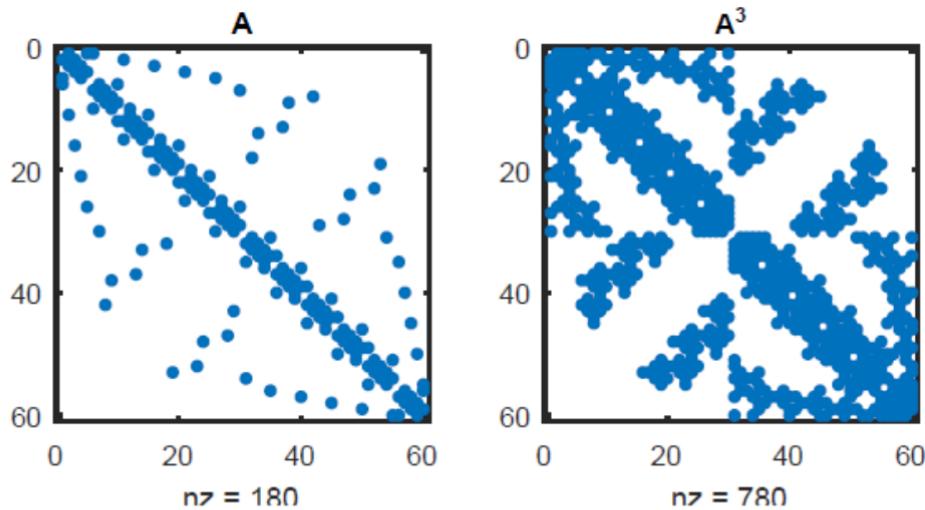


The `spy` command plots nonzero elements and gives the number of nonzeros...

Matrix fill-in

[Example 8.1.2]

Example 8.1.2



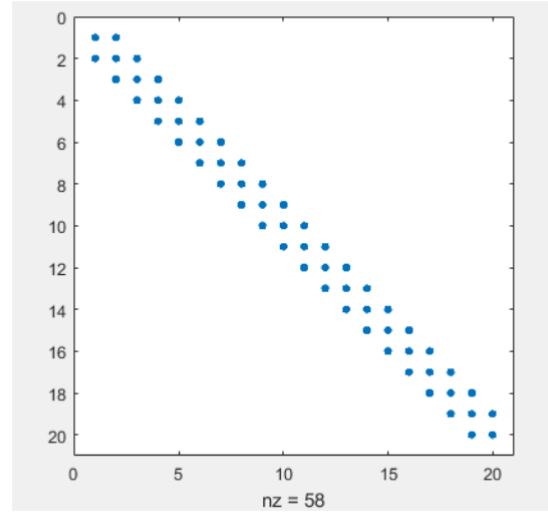
The number of nonzeros increased by more than 4x

Banded matrices

- This is an important class of matrices that comes up in applications
- The simplest is the diagonal matrix: bandwidth 1
- Another is tridiagonal, with main diagonal, as well as one superdiagonal and one subdiagonal: bandwidth is 3
- More generally, if p nonzero superdiagonals, and q nonzero subdiagonals, then bandwidth is ~~$p+q+1$~~

$$p+q+1$$

```
>> n=20;  
>> v = ones(n,1);  
>> d = [-v 2*v -0.5*v];  
>> pos = [-1 0 1];  
>> A = spdiags(d,pos,n,n);  
>> spy(A)  
>> |
```



Example: solving a banded system

Example 8.1.3

```
n = 50;
d = [ n*ones(n,1), ones(n,1), -(1:n)' ]; % diagonal entries
pos = [-3 0 1]; % which diagonals
A = spdiags(d,pos,n,n);
full( A(1:7,1:7) )
```

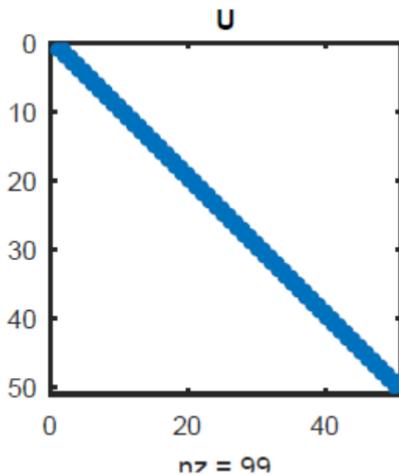
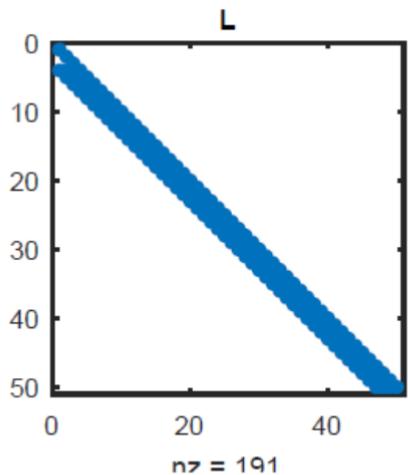
```
ans =
    1     -2      0      0      0      0      0
    0      1     -3      0      0      0      0
    0      0      1     -4      0      0      0
   50      0      0      1     -5      0      0
    0     50      0      0      1     -6      0
    0      0     50      0      0      1     -7
    0      0      0     50      0      0      1
```

- Sparse tridiagonal matrix created
- Matlab trims the size of the vectors put into the diagonals
- Full version displayed
- Solving a system?

Example: solving a banded system

Example 8.1.3

```
[L, U] = lufact(A);  
subplot(1,2,1), spy(L), title('L')  
subplot(1,2,2), spy(U), title('U')
```



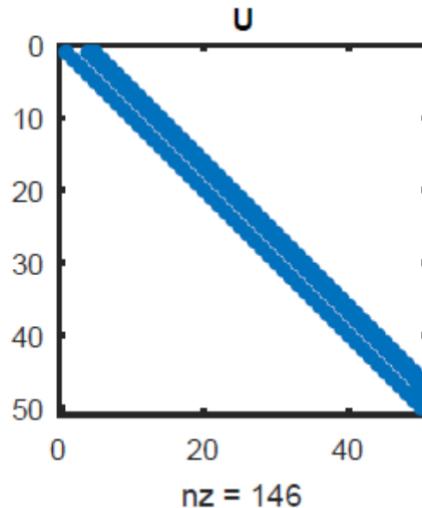
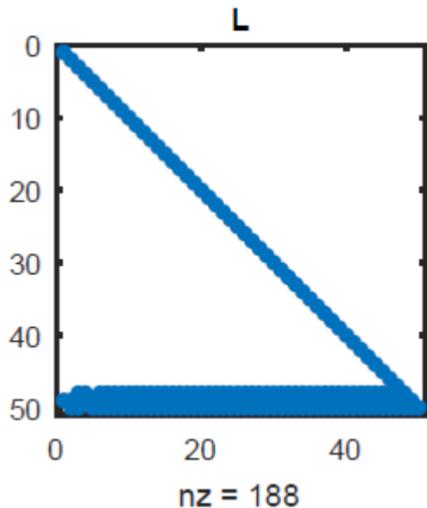
- No pivoting here
- Small bandwidth preserved

Example: solving a banded system

Example 8.1.3

```
[L,U,P] = lu(A);  
subplot(1,2,1), spy(L), title('L')  
subplot(1,2,2), spy(U), title('U')
```

[Example 8.1.3]



- Pivoting used here
- Bandwidth grows a little in U, but a lot in L to roughly $n/2$

Linear systems and eigenvalues

- Say one starts with a sparse matrix \mathbf{A} and compatible right-hand-side \mathbf{b}
- In Matlab, $\mathbf{A}\backslash\mathbf{b}$ will automatically try a sparse-aware form of Cholesky or pivoted LU factorization *Julia: multiple dispatch*
- This approach could beat the $O(n^3)$ cost for the general case with a full matrix, but this depends on the sparsity pattern of \mathbf{A}
- For a very large \mathbf{A} , it is unlikely that one would compute all of the eigenvalues and eigenvectors of \mathbf{A} , that is, one would typically not use `eig` for very large matrices *Julia: eigen, eigvals, eigs*
- For very large \mathbf{A} , one would use `eigs` (Sec 8.4) to find the a selected number of eigenvalues, often the largest or those nearest a selected complex number (the s at the end indicates sparse; there is a similar `svds` command) *Julia: svd, svdvals, svds*

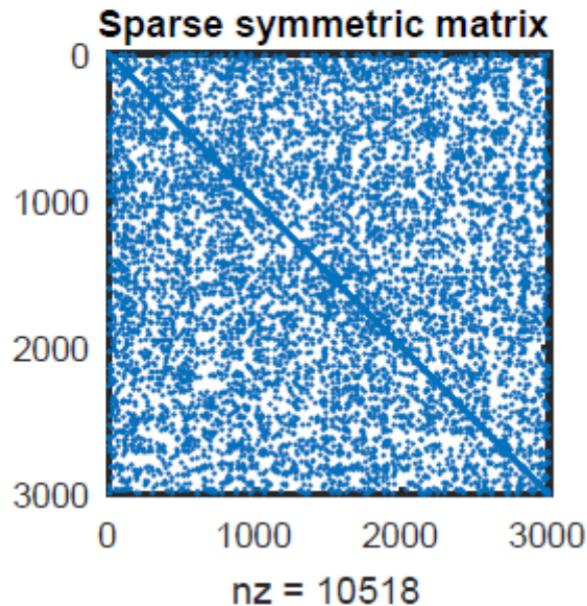
Example: sparse matrix eigenvalues

Example 8.1.4

The `sprandsym` command generates a random sparse matrix with prescribed eigenvalues.

```
n = 3000;
density = 1.23e-3;
lambda = 1./(1:n);
A = sprandsym(n,density,lambda);
spy(A)
eigs(A,5)    % largest magnitude
```

```
ans =
1.0000
0.5000
0.3333
0.2500
0.2000
```



Example: sparse matrix eigenvalues

Example 8.1.4

```
eigs(A,5,0) % closest to zero
```

```
ans =  
1.0e-03 *  
0.3338  
0.3337  
0.3336  
0.3334  
0.3333
```

[Example 8.1.4]

```
x = 1./(1:n)'; b = A*x;  
tic, sparse_err = norm(x - A\b), sparse_time = toc
```

```
sparse_err =  
2.1074e-14  
sparse_time =  
0.0110
```

- Predicting order of FLOps is difficult without info re **A**
- But sparse calculation is often faster

```
A = full(A);  
tic, dense_err = norm(x - A\b), dense_time = toc
```

```
dense_err =  
7.2768e-14  
dense_time =  
0.2792
```

Section 8.2

Power Iteration

Google Pagerank algorithm

Example: repeated matrix multiplication

Let's use that fast matrix-vector multiplication

Example 8.2.1

```
A = magic(5)/65;  
x = randn(5,1)
```

```
y = A*x
```

```
z = A*y
```

```
x =  
1.7491  
0.1326  
0.3252  
-0.7938  
0.3149
```

```
y =  
0.4864  
0.5707  
0.0473  
0.1467  
0.4770
```

```
z =  
0.4668  
0.3701  
0.2987  
0.2634  
0.3291
```

- Nothing to good happening yet
- Now try more factors of **A**

Example: repeated matrix multiplication

Example 8.2.1

```
for j = 1:8, x = A*x; end  
[x, A*x]
```

```
ans =  
0.3457 0.3457  
0.3457 0.3456  
0.3455 0.3456  
0.3455 0.3456  
0.3456 0.3456
```

```
x = randn(5,1)  
for j = 1:8, x = A*x; end  
[x, A*x]
```

- After 8 times,
we are getting
 $Ax \approx x$
- But this seems
to happen lots
of initial
vectors

```
x =  
-0.5273  
0.9323  
1.1647  
-2.0457  
-0.6444  
ans =  
-0.2240 -0.2241  
-0.2239 -0.2241  
-0.2239 -0.2241  
-0.2242 -0.2241  
-0.2243 -0.2240
```

Example: repeated matrix multiplication

Example 8.2.1

- Using eig, we find that the eigenvalues are $1, \pm 0.327, \pm 0.202$
- It turns out that we would be right to think that the process at left is converging to $Ax = \lambda x$ with $\lambda = 1$
- It turns out that this process converges to the largest eigenvalue and its associated eigenvalue ~~vector~~
- Why?

[Example 8.2.1]

```
x = randn(5,1)
for j = 1:8, x = A*x; end
[x, A*x]
```

```
x =
-0.5273
0.9323
1.1647
-2.0457
-0.6444
ans =
-0.2240 -0.2241
-0.2239 -0.2241
-0.2239 -0.2241
-0.2242 -0.2241
-0.2243 -0.2240
```

Dominant eigenvalue

- Suppose that we have an $n \times n$ diagonalizable matrix A
- The eigenvalues are $\lambda_1, \lambda_2, \dots, \lambda_n$ with associated eigenvectors v_1, v_2, \dots, v_n
- Suppose also that

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_n|.$$

- λ_1 is the dominant eigenvalue
- The v_k are an LI set, so we can express the general initial vector as a linear combo of them:

$$x = c_1 v_1 + c_2 v_2 + \cdots + c_n v_n.$$

- We know that $A v_k = \lambda_k v_k$; use that with repeated mult by A

Dominant eigenvalue

- First,

$$\begin{aligned} \mathbf{A}\mathbf{x} &= c_1 \mathbf{A}\mathbf{v}_1 + c_2 \mathbf{A}\mathbf{v}_2 + \cdots + c_n \mathbf{A}\mathbf{v}_n \\ &= c_1 \lambda_1 \mathbf{v}_1 + c_2 \lambda_2 \mathbf{v}_2 + \cdots + c_n \lambda_n \mathbf{v}_n. \end{aligned}$$

- Now use this repeatedly, factor out dominant eigenvalue

$$\begin{aligned} \mathbf{A}^k \mathbf{x} &= \lambda_1^k c_1 \mathbf{v}_1 + \lambda_2^k c_2 \mathbf{v}_2 + \cdots + \lambda_n^k c_n \mathbf{v}_n \\ &= \lambda_1^k \left[c_1 \mathbf{v}_1 + \left(\frac{\lambda_2}{\lambda_1} \right)^k c_2 \mathbf{v}_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1} \right)^k c_n \mathbf{v}_n \right]. \end{aligned}$$

- Does the left side approach $c_1 \mathbf{v}_1$? How fast?

Dominant eigenvalue

- Rewrite the equation a bit: divide by λ_1^k , and subtract $c_1 v_1$ from both sides to get

$$\frac{A^k x}{\lambda_1^k} - c_1 v_1 = \left(\frac{\lambda_2}{\lambda_1}\right)^k c_2 v_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_n v_n.$$

- Now take a norm of both sides, and use the triangle inequality:

$$\left\| \frac{A^k x}{\lambda_1^k} - c_1 v_1 \right\| \leq |c_2| \cdot \left| \frac{\lambda_2}{\lambda_1} \right|^k \|v_2\| + \cdots + |c_n| \cdot \left| \frac{\lambda_n}{\lambda_1} \right|^k \|v_n\| \rightarrow 0 \text{ as } k \rightarrow \infty.$$

- The right side tends to zero because the ratios of eigenvalues are all less than one: $A^k x$ becomes almost parallel to dominant eigenvector
- We need $c_1 \neq 0$, essentially guaranteed with random initial vector
- Important to think of this as repeated matrix vector multiplication

Power iteration

- We do repeated matrix-vector multiplication
- To make a more practical method, we also renormalize the vector with it's largest element each iteration
- Let $|y_{k,m}| = \|y_k\|_\infty$ (m is m th component)
- Note $\|x_{k+1}\|_\infty = 1$

Power iteration algorithm:

1. Choose x_1 .
2. For $k = 1, 2, \dots$

$$y_k = Ax_k,$$

$$\alpha_k = \frac{1}{y_{k,m}}, \text{ where } |y_{k,m}| = \|y_k\|_\infty,$$

$$x_{k+1} = \alpha_k y_k.$$

Note that

$$X_2 = \alpha_1 A X_1$$

$$X_3 = \alpha_2 A X_2 = \alpha_1 \alpha_2 A^2 X_1$$

⋮

$$\boxed{X_{k+1} = \alpha_1 \alpha_2 \cdots \alpha_k A^k X_1}$$

Since $y_k = Ax_k$, if $Ax_k \approx \lambda_1 x_k$,

then $y_k \approx \lambda_1 x_k$, so $\textcircled{y_{k,m}} \approx \lambda_1 x_{k,m}$.

Thus, $\boxed{\frac{y_{k,m}}{x_{k,m}} \approx \lambda_1}$. In fact,
↑ largest in abs. val.

$$\frac{y_{k,m}}{x_{k,m}} = \frac{(Ax_k)_m}{(x_k)_m} = \frac{\alpha_1 \cdots \alpha_{k-1} (A^k x_1)_m}{\alpha_1 \cdots \alpha_{k-1} (A^{k-1} x_1)_m} = \frac{(A^k x_1)_m}{(A^{k-1} x_1)_m}$$

$$= \frac{\lambda_1^k \left[c_1 v_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^k c_2 v_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^k c_n v_n \right]_m}{\lambda_1^{k-1} \left[c_1 v_1 + \left(\frac{\lambda_2}{\lambda_1}\right)^{k-1} c_2 v_2 + \cdots + \left(\frac{\lambda_n}{\lambda_1}\right)^{k-1} c_n v_n \right]_m}$$

Let $r_j = \frac{\lambda_j}{\lambda_1}$, for $j=2, \dots, n$.

Then $|r_j| < 1$, for $j=2, \dots, n$, so

$$\frac{Y_{k,m}}{X_{k,m}} = \lambda_1 \frac{[c_1 v_1 + r_2^k c_2 v_2 + \dots + r_n^k c_n v_n]_m}{[c_1 v_1 + r_2^{k-1} c_2 v_2 + \dots + r_n^{k-1} c_n v_n]_m}$$

$$\rightarrow \lambda_1 \frac{[c_1 v_1]_m}{[c_1 v_1]_m} = \lambda_1.$$

(as $k \rightarrow \infty$)

We let $\gamma_k = \frac{Y_{k,m}}{X_{k,m}}$. Then

$$\boxed{\gamma_k \rightarrow \lambda_1 \text{ as } k \rightarrow \infty.}$$

Moreover, it can be shown that

$$\boxed{\frac{\gamma_{k+1} - \lambda_1}{\gamma_k - \lambda_1} \rightarrow \frac{\lambda_2}{\lambda_1} \text{ as } k \rightarrow \infty}$$

which tells us that $\gamma_k \rightarrow \lambda_1$ at a linear rate.

Dominant eigenvalue

- What about the eigenvalue?
- k th approximation is

$$\gamma_k = \frac{y_{k,m}}{x_{k,m}} = \lambda_1 \frac{1 + r_2^{k+1} b_2 + \cdots + r_n^{k+1} b_n}{1 + r_2^k b_2 + \cdots + r_n^k b_n},$$

where $r_j = \lambda_j / \lambda_1$ and the b_j are constants.

$$r_j < 1$$

- With our ordering, ~~$\|w\|<1$~~ , and we have convergence to the dominant eigenvalue as $k \rightarrow \infty$
- Function poweriter implements this in Matlab

Function poweriter

```
1 function [gamma,x] = poweriter(A,numiter)
2 % POWERITER    Power iteration for the dominant eigenvalue.
3 % Input:
4 % A            square matrix
5 % numiter     number of iterations
6 % Output:
7 % gamma       sequence of eigenvalue approximations (vector)
8 % x           final eigenvector approximation
9
10 n = length(A);
11 x = randn(n,1);
12 x = x/norm(x,inf);
13 for k = 1:numiter
14     y = A*x;
15     [normy,m] = max(abs(y));
16     gamma(k) = y(m)/x(m);
17     x = y/y(m);
18 end
```



- max returns max value and location in vector
- Sparsity used automatically

Convergence of power iteration

- Return to k th approximation:

$$\gamma_k = \frac{y_{k,m}}{x_{k,m}} = \lambda_1 \frac{1 + r_2^{k+1} b_2 + \cdots + r_n^{k+1} b_n}{1 + r_2^k b_2 + \cdots + r_n^k b_n},$$

where $r_j = \lambda_j / \lambda_1$ and the b_j are constants.

- Consider the denominator:

$$\begin{aligned} r_2^k b_2 + \cdots + r_n^k b_n &= r_2^k \left[b_2 + \left(\frac{r_3}{r_2} \right)^k b_3 + \cdots + \left(\frac{r_n}{r_2} \right)^k b_n \right] \\ &= r_2^k \left[b_2 + \left(\frac{\lambda_3}{\lambda_2} \right)^k b_3 + \cdots + \left(\frac{\lambda_n}{\lambda_2} \right)^k b_n \right]. \end{aligned}$$

- For simplicity, assume that

$$|\lambda_2| > |\lambda_3| \geq \cdots \geq |\lambda_n|.$$

Convergence of power iteration

- With this assumption all of the ratios $\left(\frac{r_j}{r_2}\right)^k \rightarrow 0$ for $k \rightarrow \infty$, so that the term approaches just the leading term, $b_2 r_2^k$, for large k
- With the simpler denominator, it is relatively easy to use a geometric series for it
- Using that in the eigenvalue approximation gives

$$\gamma_k \rightarrow \lambda_1 \left(1 + b_2 r_2^{k+1}\right) \left(1 - b_2 r_2^k + O(r_2^{2k})\right),$$
$$\gamma_k - \lambda_1 \rightarrow \lambda_1 b_2 (r_2 - 1) r_2^k.$$

- The next term has $\gamma_{k+1} - \lambda_1 \rightarrow \lambda_1 b_2 (r_2 - 1) r_2^{k+1}$
- Dividing the last two expressions tells us what happens each iteration...

Convergence of power iteration

- We find that the ratio is

$$\frac{\gamma_{k+1} - \lambda_1}{\gamma_k - \lambda_1} \rightarrow r_2 = \frac{\lambda_2}{\lambda_1} \quad \text{as } k \rightarrow \infty.$$

r_2

- The new approximation is roughly a factor of $\frac{r_2}{\lambda_1}$ closer than the old one
- This is linear convergence: the error drops by a constant factor each time
- It is usually true once one has done a few iterations, so that the computed values start to come from “large k ”
- Thinking of taking this limit for a (potentially) large number of iterations is what we mean when we say:

The error in the eigenvalue estimates γ_k of power iteration is reduced asymptotically by a constant factor λ_2/λ_1 on each iteration.

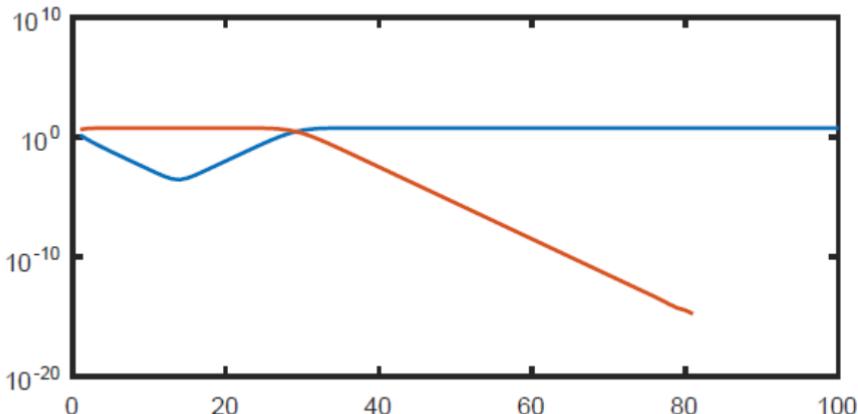
Example: convergence

[Example 8.2.2]

Example 8.2.2

```
A= [ 6 3 3; 1 10 1; 2 5 5];
[V,D] = eig(A);
x = [2;-1;2]+1e-8;
for n = 1:100
    y = A*x;
    [~,m] = max(abs(y));
    gamma(n) = y(m)/x(m);
    x = y/y(m);
end
semilogy(abs(gamma-6))
hold on, semilogy(abs(gamma-12))
```

- How fast do iterates gamma converge to eigenvalues?
- Blue: $\lambda_2 = 6$; red: $\lambda_1 = 12$
- Linear convergence to λ_1



Convergence of power iteration

- This is not a practical implementation
- We will continue to improved methods

Section 8.3

Inverse Iteration

Inverse iteration

- Power iteration only finds the dominant eigenvalue
- We can extend power iteration to find other eigenvalues
- The idea is to use some simple linear algebra results to change the relative sizes of the eigenvalues

Inverse iteration

- Here are those linear algebra results

Theorem 8.3.1

Let A be an $n \times n$ matrix with eigenvalues $\lambda_1, \dots, \lambda_n$ (possibly with repeats), and let s be a complex scalar. Then:

1. The eigenvalues of the matrix $A - sI$ are $\lambda_1 - s, \dots, \lambda_n - s$.
2. If s is not an eigenvalue of A , the eigenvalues of the matrix $(A - sI)^{-1}$ are $(\lambda_1 - s)^{-1}, \dots, (\lambda_n - s)^{-1}$.
3. The eigenvectors associated with the eigenvalues in the first two parts are the same as those of A .

Inverse iteration

- Great options for moving around eigenvalues, if true
- Consider item 1: start with $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$; subtract $s\mathbf{I}\mathbf{v}$ from both sides

$$\begin{aligned}\mathbf{A}\mathbf{v} - s\mathbf{I}\mathbf{v} &= \lambda\mathbf{v} - s\mathbf{I}\mathbf{v} \rightarrow \\ (\mathbf{A} - s\mathbf{I})\mathbf{v} &= (\lambda - s)\mathbf{v}\end{aligned}$$

- We have that a matrix times a vector gives a scalar times the same vector, as in part 1: proven.
- For part 2, we assumed that $s \neq \lambda_k$, so $\mathbf{A} - s\mathbf{I}$ is non-singular, then straightforward rearrangement gives
$$(\mathbf{A} - s\mathbf{I})^{-1}\mathbf{v} = (\lambda_k - s)^{-1}\mathbf{v}$$
- This proves that item 2 is true.
- Item 3 follows too.

Inverse iteration

- Consider item 2 with $s = 0$: start with A having a *smallest eigenvalue*:

$$|\lambda_n| \geq |\lambda_{n-1}| \geq \cdots > |\lambda_1|.$$

- Then

$$|\lambda_1^{-1}| > |\lambda_2^{-1}| \geq \cdots \geq |\lambda_n^{-1}|,$$

so that the reciprocal of *the smallest eigenvalue* is now the dominant one

- We can use power iteration to find the reciprocal value, and thus approximate the smallest eigenvalue (the one closest to zero)
- This is *inverse iteration*
- The convergence rate is linear again, with rate

$$\frac{\lambda_2^{-1}}{\lambda_1^{-1}} = \frac{\lambda_1}{\lambda_2}.$$

Shifted inverse iteration

- Consider $s \neq 0$: order eigenvalues of $\mathbf{A} - s\mathbf{I}$ with distance from s

$$|\lambda_n - s| \geq \dots \geq |\lambda_2 - s| > |\lambda_1 - s|,$$

- Then

$$|\lambda_1 - s|^{-1} > |\lambda_2 - s|^{-1} \geq \dots \geq |\lambda_n - s|^{-1}.$$

- We can use power iteration to find the first reciprocal value, and thus approximate the eigenvalue closest to s
- This is *shifted inverse iteration*
- Power iteration on $(\mathbf{A} - s\mathbf{I})^{-1}$ converges to $(\lambda_1 - s)^{-1}$ provided that λ_1 is closest to s

Shifted inverse iteration

- There is a new computational wrinkle here
- We want to find: $y_k = (A - sI)^{-1}x_k$. for a sequence of k values
- However, we do NOT want to compute $(A - sI)^{-1}$ to do it!
- Instead, we could write what is needed as

Solve $(A - sI)y_k = x_k$ for y_k .

- The solve is the computational version of the inverse, but is faster !!!

Shifted inverse iteration

- We need

Solve $(A - sI)y_k = x_k$ for y_k .

$$y = \underbrace{(A - sI) \setminus x}_{\text{C will factor } A - sI \text{ each time}}$$

- To begin with, we use PLU factorization, and live with any fill-in that may result for sparse matrices
- Function 8.3.1 does inverse iteration
- Note that the iteration is for $\beta_k = (\gamma_k - s)^{-1}$; the approximation to the original eigenvalue is $\gamma_k = s + \beta_k^{-1}$

Function inviter

Function 8.3.1 (inviter) Shifted inverse iteration for the closest eigenvalue.

```
1 function [gamma,x] = inviter(A,s,numiter)
2 % INVITER    Shifted inverse iteration for the closest eigenvalue.
3 % Input:
4 %   A          square matrix
5 %   s          value close to targeted eigenvalue (complex scalar)
6 %   numiter    number of iterations
7 % Output:
8 %   gamma      sequence of eigenvalue approximations (vector)
9 %   x          final eigenvector approximation
10
11 n = length(A);
12 x = randn(n,1);
13 x = x/norm(x,inf);
14 B = A - s*eye(n); ←
15 [L,U] = lu(B);
16 for k = 1:numiter
17     y = U \ (L\x);
18     [normy,m] = max(abs(y));
19     gamma(k) = x(m)/y(m) + s;
20     x = y/m;
21 end
```

- Random x ensures some component in eigenvector direction
- Should be $s * speye(n)$ here

Example: inverse iteration

Example 8.3.1

```
lambda = [1 -0.75 0.6 -0.4 0];
A = triu(ones(5),1) + diag(lambda);
format long

[gamma, x] = inviter(A, 0.7, 30);
eigval = gamma(end)

eigval =
    0.599999999999998
```

- Create a 5×5 matrix with known eigenvalues
- Use $s = 0.7$ and do 30 iterations
- Convergence is to closest eigenvalue with value 0.6

Example: inverse iteration

Example 8.3.1

```
observed_rate = err(26)/err(25)
```

```
observed_rate =
-0.327983951855567
```

```
theoretical_rate = (lambda(3)-0.7) / (lambda(1)-0.7)
```

```
theoretical_rate =
-0.3333333333333333
```

- We could also compute the ratio $(\gamma_{k+1} - s)/(\gamma_k - s)$ in Matlab using $s=0.7$ and

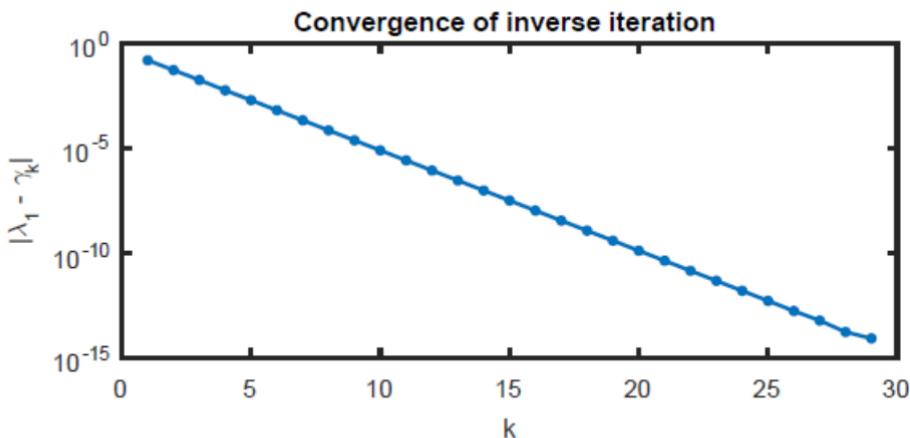
```
seq_of_rate = (gamma(2:end)-s)./(gamma(1:end-1)-2)
```

and see that the sequence of ratios approaches $1/3$

Example: inverse iteration

Example 8.3.1

```
err = eigval - gamma;  
semilogy(abs(err), '.-')
```



- Convergence rate is linear: drops by constant factor of about 0.33 each time
- How do we know this?

[Example 8.3.1]

Dynamic shifting

- In our last example, we left s as a single value throughout the iteration
- This works reasonably well, but one can do better
- This time, let $s = \gamma_k$ when we compute γ_{k+1}
- So, we are adjusting s on the fly
- How well does it work?

Example: inverse iteration

Example 8.3.2

```
lambda = [1 -0.75 0.6 -0.4 0];
A = triu(ones(5),1) + diag(lambda);
format long
I = eye(5); s = 0.7;
x = ones(5,1);
y = (A-s*I)\x; gamma = x(1)/y(1) + s
```

```
gamma =
0.703481392557023
```

```
s = gamma;
x = y/y(1);
y = (A-s*I)\x; gamma = x(1)/y(1) + s
```

```
gamma =
0.561276140617300
```

- Same 5×5 matrix as previous example
- Use $s = 0.7$ and do 1 iteration
- Change s to γ and repeat
- Doesn't look too good yet, but...

Example: inverse iteration

Example 8.3.2

```
for k = 1:4
    s = gamma; x = y/y(1);
    y = (A-s*I)\x; gamma = x(1)/y(1) + s
end
```

```
gamma =
0.596431288475387
gamma =
0.599971709182010
gamma =
0.599999997855635
gamma =
0.6000000000000000
```

- Now repeat the process a few times
- Boom!
- Convergence is very rapid: roughly double the number of digits each time
- This is *quadratic convergence*
- Like Newton's method near a root

[Example 8.3.2]

Dynamic shifting

- There is a price for this increased rate of convergence
- Before, with constant shift, we could factor $A - sI$ once, and each iterate is faster, but there can be many more
- With dynamic shifting, we need to factor $A - s_k I$ for each iteration but there may be many fewer iterations
- For our examples, 30 iterates for constant shift, only 6 with dynamic shift
- In many cases it pays off to dynamically shift.

Section 8.4

Krylov Subspaces

Krylov subspaces

$$A \in \mathbb{R}^{n \times n}$$
$$Ax = b$$

- Say we start with a seed vector \mathbf{u}
- If we repeatedly multiply by a matrix A , we can keep all of the products, and try to use that set as a basis for approximating answers.
- Thus, we are creating the set $\mathbf{u}, A\mathbf{u}, A^2\mathbf{u}, \dots, A^{n-1}\mathbf{u} \in \mathbb{R}^n$
- In the power or inverse iterations we only kept the latest on each time $x \in \mathbb{R}^n \Rightarrow x = z_1\mathbf{u} + z_2A\mathbf{u} + \dots + z_n A^{n-1}\mathbf{u}$
- We get the $n \times m$ Krylov matrix if the columns are $\mathbf{u}, A\mathbf{u}, A^2\mathbf{u}, \dots$

$$K_m = [\mathbf{u} \quad A\mathbf{u} \quad A^2\mathbf{u} \quad \dots \quad A^{m-1}\mathbf{u}]$$

Krylov subspaces

$$A^2 = A \quad A^k = A \quad A = I$$

- The columns of the $n \times m$ Krylov matrix are important

$$K_m = [u \quad Au \quad A^2u \quad \cdots \quad A^{m-1}u]$$

- The columns form the m th Krylov subspace \mathcal{K}_m of \mathbb{C}^n
- Each column is n long, but there are only m columns
- We want to approximate answers from this subspace; said another way, we want to find answers that are a linear combo of the columns
- The dimension of \mathcal{K}_m is the same as the rank of K_m , which is often m but may be smaller

Properties

- Generating columns of Krylov matrix is relatively easy for sparse A

$$K_m = [u \quad Au \quad A^2u \quad \dots \quad A^{m-1}u]$$

- And, there are some nice properties...

Lemma 8.4.1

Suppose A is $n \times n$, $0 < m < n$, and a vector u is used to generate Krylov subspaces. If $x \in \mathcal{K}_m$, then the following hold:

- $x = K_m z$ for some $z \in \mathbb{C}^m$
$$x = z_1 u + z_2 A u + \dots + z_m A^{m-1} u$$
- $x \in \mathcal{K}_{m+1}$
$$x = z_1 u + z_2 A u + \dots + z_m A^{m-1} u + 0 \cdot A^m u \quad (z_{m+1} = 0)$$
- $Ax \in \mathcal{K}_{m+1}$

$$\mathcal{K}_m \subseteq \mathcal{K}_{m+1}$$

$$Ax = 0 \cdot u + z_1 A u + z_2 A^2 u + \dots + z_m A^m u$$

Properties

- Part 1 simply says that if $x \in \mathcal{K}_m$, then for some coefficients c_1, c_2, \dots, c_m , x can be written as

$$x = c_1 u + c_2 A u + \cdots + c_m A^{m-1} u.$$

- Then, let $z = [c_1 \ c_2 \ \dots \ c_m]^T$, and recall that

$$K_m = [u \ \ A u \ \ A^2 u \ \ \cdots \ \ A^{m-1} u]$$

- For Part 3, just multiply the first equation by A , and one has

$$Ax = c_1 A u + c_2 A^2 u + \cdots + c_m A^m u \in \mathcal{K}_{m+1}.$$

Reducing dimension and solving linear systems

- Consider the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ for $n \times n$ nonsingular \mathbf{A}
- The original idea for using Krylov subspaces was to create a space with n basis vectors, $\mathcal{K}_n = \mathbb{R}^n$
- This could come with a predetermined number of steps, making it a direct method ($m = n$ here for multiplications by \mathbf{A})

$$\mathbf{K}_m = [\mathbf{u} \quad \mathbf{A}\mathbf{u} \quad \mathbf{A}^2\mathbf{u} \quad \cdots \quad \mathbf{A}^{m-1}\mathbf{u}]$$

- However, the columns of K_m effectively come from power method
- The columns are converging to the dominant eigenvector
- This makes the *direct method* with $m = n$ ill-conditioned and impractical

Reducing dimension and solving linear systems

- An alternative view is to say that most of the approximation or information is in the first few columns; the farther out columns are nearly dependent
- Why not stop early and perhaps get a good approximation with only $m < n$ basis vectors, that is, \mathcal{K}_m
- The problem changes then to one where we don't know in advance when to stop: it becomes an iterative method.
- Also, we need to get the best answer for the system $Ax = b$ with n unknowns: this suggests a minimization of the error:

$$\min_{\mathbf{x} \in \mathcal{K}_m} \|A\mathbf{x} - \mathbf{b}\| = \min_{\mathbf{z} \in \mathbb{C}^m} \|A(K_m \mathbf{z}) - \mathbf{b}\| = \min_{\mathbf{z} \in \mathbb{C}^m} \|(AK_m)\mathbf{z} - \mathbf{b}\|.$$

Reducing dimension and solving linear systems

- For the linear system $Ax = \mathbf{b}$, the natural choice to start the Krylov iteration is $\mathbf{u} = \mathbf{b}$

$$K_m = [u \quad Au \quad A^2u \quad \dots \quad A^{m-1}u]$$

- We do adjust the size of each column with a normalization to prevent wildly different sizes of the elements
- Let's do an example

Example: Krylov iteration

Example 8.4.1

```
% Create a triangular matrix with  
% known eigenvalues and a random vector b  
lambda = 10 + (1:100) ;  
A = diag( lambda ) + triu( rand(100),1 );  
b = rand(100 ,1) ;  
  
% Next we build up the first thirty Krylov  
% matrices iteratively, using renormalization  
% after each matrix-vector multiplication.  
Km = b;  
for m = 1:29  
    v = A*Km(:,m);  
    Km(:,m+1) = v/norm(v);  
end
```

[Example 8.4.1]

- m th column of K_m created each time
- Normalize the column and append it

Example: Krylov iteration

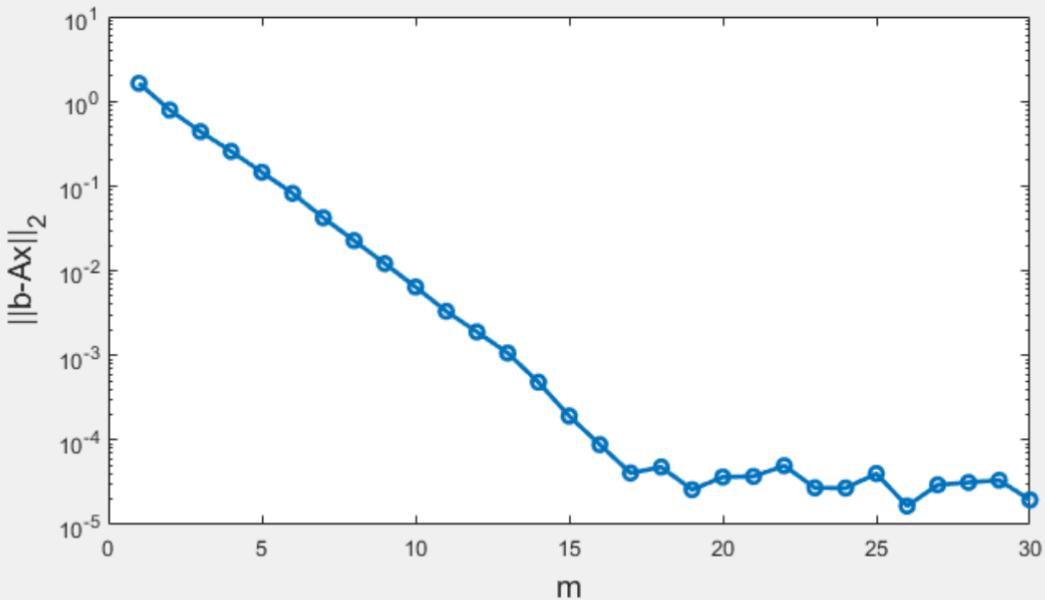
Example 8.4.1

```
% Now we solve a least squares problem for  
% Krylov matrices of increasing dimension.  
for m = 1:30  
    z = ( A*Km(:,1:m) )\b;  
    x = Km(:,1:m)*z;  
    resid(m) = norm( b-A*x );  
end  
  
% The linear system approximations show smooth  
% linear convergence at first, but  
% the convergence stagnates after only a  
% few digits have been found.  
semilogy(resid,'o-','LineWidth',2)  
ylabel('||b-Ax||_2','FontSize',14)  
xlabel('m','FontSize',14)
```

- Use the first m columns of K_m to approximate the solution
- \ does least squares solution here
- Compute and save the residual

Example: Krylov iteration

Example 8.4.1



- Residual “stalls” at $m=17$
- Matlab throws warnings at that point because K_m is nearly singular
- We need a better approach!

Fixing the problem

- The Krylov matrix we were generating was for $m = 30$ with

$$K_m = [u \quad Au \quad A^2u \quad \dots \quad A^{m-1}u]$$

- After column 17, any new columns were nearly dependent on the previous ones: warnings for $m \geq 17$
- The opposite of this problem is to use an orthogonal matrix, where the columns are far from dependent
- Try QR factorization:

$$K_m = \text{span}\{q_1, \dots, q_m\}$$

$$K_m = Q_m R_m = [q_1 \quad q_2 \quad \dots \quad q_m] \begin{bmatrix} R_{11} & R_{12} & \cdots & R_{1m} \\ 0 & R_{22} & \cdots & R_{2m} \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & R_{mm} \end{bmatrix}$$

Fixing the problem

- The columns $\mathbf{q}_j, j = 1, \dots, m$ of \mathbf{Q} are orthonormal
- And, they are a basis for \mathcal{K}_m !
- From Lemma 8.4.1, we know that multiplying a vector in \mathcal{K}_m with A will produce a vector in \mathcal{K}_{m+1}
- Using the last column of \mathbf{Q} , we know that

$$A\mathbf{q}_m \in \mathcal{K}_{m+1} = \text{span}\{\mathbf{q}_1, \dots, \mathbf{q}_{m+1}\}$$

- It's then a linear combo of the $m + 1$ columns of another \mathbf{Q} :

$$A\mathbf{q}_m = H_{1m}\mathbf{q}_1 + H_{2m}\mathbf{q}_2 + \cdots + H_{m+1,m}\mathbf{q}_{m+1},$$

Fixing the problem

$$q_i^*(Aq_m) = 0 + 0 + \cdots + q_i^* H_{im} q_i + \cdots +$$

- Because the columns q_j are orthonormal,

$$q_i^* q_j = 0, \quad i \neq j$$

$$q_i^* q_j = 1, \quad i = j$$

- Premultiply by q_i^* , and only one term on the right survives:

$$q_i^* (Aq_m) = H_{1m} q_1 + H_{2m} q_2 + \cdots + H_{m+1,m} q_{m+1}$$

- We get $q_i^*(Aq_m) = H_{im}$, $i = 1, \dots, m$ $H_{im} = q_i^*(Aq_m)$

- Orthonormality of the q_j makes this easy!!

- The first m q_j are known, and the H_{im} are then determined.

- What about the last term on the right?

Fixing the problem: Arnoldi iteration

- With the first m \mathbf{q}_j are known, and the H_{im} found, we can rearrange:

$$V = H_{m+1,m} \mathbf{q}_{m+1} = A\mathbf{q}_m - \sum_{i=1}^m H_{im} \mathbf{q}_i$$
$$H_{m+1,m} = \|V\|$$
$$\mathbf{q}_{m+1} = \frac{V}{\|V\|}$$

- Now, we only know $H_{m+1,m} \mathbf{q}_{m+1}$
- However, we know that we want \mathbf{q}_{m+1} to be a *unit vector*
- So, we can make $H_{m+1,m}$ the norm of the result, and make \mathbf{q}_{m+1} its direction.
- This is called *Arnoldi iteration*

$$H_{im} = q_i^*(A\mathbf{q}_m), \quad i=1, \dots, m$$

Arnoldi iteration

- Here's an algorithm

1. Let $q_1 = u/\|u\|$.
2. For $m = 1, 2, \dots$
 - i. Use (8.4.4) to find H_{im} for $i = 1, \dots, m$.
 - ii. Let

$$v = (Aq_m) - H_{1m} q_1 - H_{2m} q_2 - \cdots - H_{mm} q_m.$$

$$H_{im} = q_i^*(Aq_m)$$

- iii. Let $H_{m+1,m} = \|v\|$.
 - iv. Let $q_{m+1} = v/H_{m+1,m}$.
- The big improvement here is that the Arnoldi algorithm finds an orthonormal basis for the Krylov subspace

Example: Arnoldi iteration

Example 8.4.2

[Example 8.4.2]

Make a few steps of Arnoldi iteration for a small matrix

```
% A few steps of Arnoldi iteration using a small matrix
A = magic(6) ;

% The seed vector determines the first member of the orthonormal basis.
u = randn(6 ,1);
Q = u/norm(u);

% Multiplication by A gives us a new vector in K2.
Aq = A*Q(:,1);

% We subtract off its projection in the previous direction.
% The remainder is rescaled to give us the next orthonormal column.
v = Aq-(Q(:,1) '*Aq)*Q(:,1);
Q(:,2) = v/norm (v)
```

- The first column was the unit vector in the u direction
- The second vector is A times that first vector, then normalized

Example: Arnoldi iteration

Example 8.4.2

```
% On the next pass, we have to subtract off  
% the projections in two previous directions.  
Aq = A*Q(:,2);  
v = Aq - (Q(:,1)'*Aq)*Q(:,1) - (Q(:,2)'*Aq)*Q(:,2)  
Q(:,3) = v/norm(v)  
  
% At every step, Qm is an ONC matrix.  
norm ( Q'*Q - eye(3) )  
  
% And Qm spans the same space as the 3-dimensional Krylov matrix.  
K = [ u A*u A*A*u ];  
rank ( [Q,K] )
```

Make a few steps of Arnoldi iteration for a small matrix

```
Q =  
-0.7836 -0.3993 0.0892  
0.2807 0.2386 0.5703  
0.2801 -0.4678 0.0839  
0.1849 0.2795 -0.2166  
0.3077 -0.3680 -0.6645  
-0.3161 0.5927 -0.4138  
  
ans =  
2.5117e-16  
ans =  
3
```

A Key Identity

- We focused on the q_j so far, but the H_{im} are important too
- They can be assembled into an *upper Hessenberg matrix*:

$$AQ_m = [Aq_1 \quad \cdots \quad Aq_m]$$

$n \times n \quad n \times m$

$$= [q_1 \quad q_2 \quad \cdots \quad q_{m+1}] \begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1m} \\ H_{21} & H_{22} & \cdots & H_{2m} \\ & H_{32} & \ddots & \vdots \\ & & \ddots & H_{mm} \\ & & & H_{m+1,m} \end{bmatrix} = Q_{m+1}H_m,$$

$n \times (m+1)$

$(m+1) \times m$

$$\boxed{AQ_m = Q_{m+1}H_m} \quad !!!$$

- This is a fundamental identity for Krylov subspace methods
- We will study practical and widely used methods based on it

Function 8.4.1 (arnoldi) Arnoldi iteration for Krylov subspaces.

```
1 function [Q,H] = arnoldi(A,u,m)
2 % ARNOLDI    Arnoldi iteration for Krylov subspaces.
3 % Input:
4 %   A      square matrix (n by n)
5 %   u      initial vector
6 %   m      number of iterations
7 % Output:
8 %   Q      orthonormal basis of Krylov space (n by m+1)
9 %   H      upper Hessenberg matrix, A*Q(:,1:m)=Q*D (m+1 by m)
10
11 n = length(A);
12 Q = zeros(n,m+1);
13 H = zeros(m+1,m);
14 Q(:,1) = u/norm(u);
15 for j = 1:m
16     % Find the new direction that extends the Krylov subspace.
17     v = A*Q(:,j);
18     % Remove the projections onto the previous vectors.
19     for i = 1:j
20         H(i,j) = Q(:,i)'*v;
21         v = v - H(i,j)*Q(:,i);
22     end
23     % Normalize and store the new basis vector.
24     H(j+1,j) = norm(v);
25     Q(:,j+1) = v/H(j+1,j);
26 end
```

Section 8.5

GMRES

GMRES: Using Arnoldi iteration

- Arnoldi iteration may be most widely used to solve the square linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ for n unknowns \mathbf{x}
- The Krylov basis (columns of K_m) was bad because some of the basis vectors were nearly dependent
- We tried to solve

$$\min_{\mathbf{x} \in \mathcal{K}_m} \|\mathbf{A}\mathbf{x} - \mathbf{b}\| = \min_{\mathbf{z} \in \mathbb{C}^m} \|\mathbf{A}K_m \mathbf{z} - \mathbf{b}\|,$$

- But, we found trouble when m got bigger
- We then went to an orthonormal basis from the QR factorization

$$K_m = Q_m R_m$$

GMRES: Using Arnoldi iteration

- Use the orthonormal columns of \mathbf{Q}_m as the basis for the approximate answer: $\mathbf{x} = \mathbf{Q}_m \mathbf{z}$ for n unknowns \mathbf{x}
- Then we have converted the problem to

$$\min_{\mathbf{z} \in \mathbb{C}^m} \|A\mathbf{Q}_m \mathbf{z} - \mathbf{b}\|.$$

- At this point, there are n equations for the m coefficients in \mathbf{z}
- To make the method efficient, we can make the system smaller:
use $A\mathbf{Q}_m = \mathbf{Q}_{m+1}\mathbf{H}_m$
- Then we have

$$\min_{\mathbf{z} \in \mathbb{C}^m} \|\mathbf{Q}_{m+1}\mathbf{H}_m \mathbf{z} - \mathbf{b}\|.$$

GMRES: Using Arnoldi iteration

- This system still has n equations for the m coefficients in \mathbf{z}

$$\min_{\mathbf{z} \in \mathbb{C}^m} \|Q_{m+1}H_m \mathbf{z} - \mathbf{b}\|.$$

- Note that \mathbf{b} is a multiple of the unit vector \mathbf{q}_1 ; we can then write

$$\mathbf{b} = \|\mathbf{b}\| \mathbf{Q}_{m+1} \mathbf{e}_1$$

- Now substitute for \mathbf{b} , to get the new problem

$$\min_{\mathbf{z} \in \mathbb{C}^m} \|Q_{m+1}(H_m \mathbf{z} - \|\mathbf{b}\| \mathbf{e}_1)\|. = \|H_m \mathbf{z} - \|\mathbf{b}\| \mathbf{e}_1\|$$

- Is this better? It is still n equations for the m coefficients in \mathbf{z}

- But, for $w \in \mathbb{C}^{m+1}$, we have

$$\|Q_{m+1}w\|^2 = w^* Q_{m+1}^* Q_{m+1} w = w^* w = \|w\|^2.$$

GMRES: Using Arnoldi iteration

- These orthogonal matrices don't change the norm!
- We need only minimize the smaller system without the Q_{m+1}

Thus

$$\min_{\mathbf{z} \in \mathbb{C}^m} \|Q_{m+1}(H_m \mathbf{z} - \|b\|e_1)\|.$$

becomes

$$\min_{\mathbf{z} \in \mathbb{C}^m} \|H_m \mathbf{z} - \|b\|e_1\|,$$

- Is this better? Now only $(m + 1)$ eqns for the m coefficients in \mathbf{z}
- The solution for this system is \mathbf{z}_m
- The solution to the original system is approximately $\mathbf{x}_m = Q_m \mathbf{z}_m$

GMRES: Using Arnoldi iteration

- This method is called GMRES, for Generalized Minimum RESidual

$$\min_{z \in \mathbb{C}^m} \|H_m z - \|b\|e_1\|,$$

$$x_m = Q_m z_m$$

- GMRES uses the output of the Arnoldi iteration to minimize the residual of $Ax = b$ over successive Krylov subspaces.
- Let's look at an example

Example: GMRES

Example 8.5.1

[Example 8.5.1]

```
lambda = 10 + (1:100);
A = diag(lambda) + triu(rand(100),1);
b = rand(100,1);

[Q,H] = arnoldi(A,b,60);

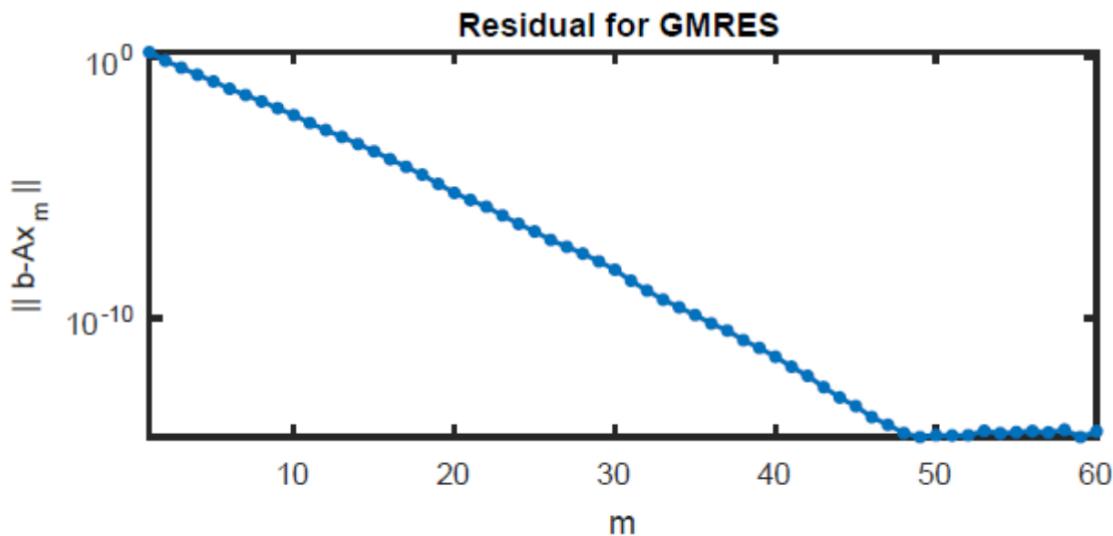
for m = 1:60
    s = [norm(b); zeros(m,1)];
    z = H(1:m+1,1:m)\s;
    x = Q(:,1:m)*z;
    resid(m) = norm(b-A*x);
end

semilogy(resid, '.-')
```

- Matrix with known eigenvalues and random b
- K_m not used, created Q, H instead
- Create a sequence of 60 approximations using one more column each time
- Plot all the residuals

Example: GMRES

Example 8.5.1



- Error drops to nearly machine epsilon before 50 columns
- No stalling of the error here

GMRES

- A basic version of the algorithm is implemented in Function 8.5.1

Function 8.5.1 (arngmres) GMRES for a linear system.

```
1 function [x,residual] = arngmres(A,b,M)
2 % ARNGMRES    GMRES for a linear system (demo only).
3 % Input:
4 %   A          square matrix (n by n)
5 %   b          right-hand side (n by 1)
6 %   M          number of iterations
7 % Output:
8 %   x          approximate solution (n by 1)
9 %   r          history of norms of the residuals
10
11 n = length(A);
12 Q = zeros(n,M);
13 Q(:,1) = b/norm(b);
14 H = zeros(M,M-1);
15
16 % Initial "solution" is zero.
17 residual(1) = norm(b);
18
```

GMRES

- A basic version of the algorithm is implemented in Function 8.5.1

```
18
19  for m = 1:M
20
21    % Next step of Arnoldi iteration.
22    v = A*Q(:,m);
23    for i = 1:m
24      H(i,m) = Q(:,i)'*v;
25      v = v - H(i,m)*Q(:,i);
26    end
27    H(m+1,m) = norm(v);
28    Q(:,m+1) = v/H(m+1,m);
29
30    % Solve the minimum residual problem.
31    r = norm(b)*eye(m+1,1);
32    z = H(1:m+1,1:m) \ r;
33    x = Q(:,1:m)*z;
34    residual(m+1) = norm( A*x - b );
35
36  end
```

- Matlab has a more sophisticated version:
gmres

GMRES: convergence and restarting

- The residual $\|r_m\| = \|\mathbf{b} - \mathbf{A}\mathbf{x}_m\|$ can't increase during Arnoldi iteration because minimization over the largest space includes the previous ones
- But, it is difficult to say more than that.
- The previous example showed the cleanest behavior.
- It turns out that phases of sublinear and superlinear convergence can happen in (typically larger) systems. This depends on the spectrum of the matrix.
- Also, the number of columns of \mathbf{Q} and the number of entries in \mathbf{H}_m : work and storage grow like m^2 , which can be too much
- Using GMRESS with *restarting* can help

GMRES: convergence and restarting

- Good things about restarting:
 - one does not lose the previous gain of getting close to the answer
 - one uses low dimensional approximations again so that memory used is never allowed to get too large
- However, the low dimensional approximations may retard or even stagnate progress
- Matlab's GMRES function allows restarting
- Number of restarts (including initial): *outer iterations*
- Number of iterations after restarting: *inner iterations*

Example: GMRES with restarting

Example 8.5.2

```
maxit = 120; rtol = 1e-8;  
d = 50;  
A = d^2*gallery('poisson',d);  
n = size(A,1)  
b = ones(n,1);  
  
n =  
    2500
```

- Matrix discretizing a PDE that will be used not uncommonly
- The name comes from the PDE problem: Poisson equation
- From built-in gallery function
- Gives a large matrix

[Example 8.5.2]

IterativeSolvers.jl

Example: GMRES with restarting

Example 8.5.2

- We use these five input arguments

```
>> help gmres
gmres    Generalized Minimum Residual Method.
X = gmres(A,B) attempts to solve the system of linear equations A*X = B
for X.  The N-by-N coefficient matrix A must be square and the right
hand side column vector B must have length N. This uses the unrestarted
method with MIN(N,10) total iterations.

X = gmres(A,B,RESTART) restarts the method every RESTART iterations.
If RESTART is N or [] then gmres uses the unrestarted method as above.

X = gmres(A,B,RESTART,TOL) specifies the tolerance of the method. If
TOL is [] then gmres uses the default, 1e-6.

X = gmres(A,B,RESTART,TOL,MAXIT) specifies the maximum number of outer
iterations. Note: the total number of iterations is RESTART*MAXIT. If
MAXIT is [] then gmres uses the default, MIN(N/RESTART,10). If RESTART
is N or [] then the total number of iterations is MAXIT.
```

Example: GMRES with restarting

Example 8.5.2

- We use these five input arguments

```
X = gmres(A,B,RESTART,TOL,MAXIT)
```

Matrix A

RHS b

Specifies tolerance
for method (1e-6
default)

Restart after
RESTART *inner*
iterations

MAXIT specifies
limit for *outer*
iterations

Example: GMRES with restarting

Example 8.5.2

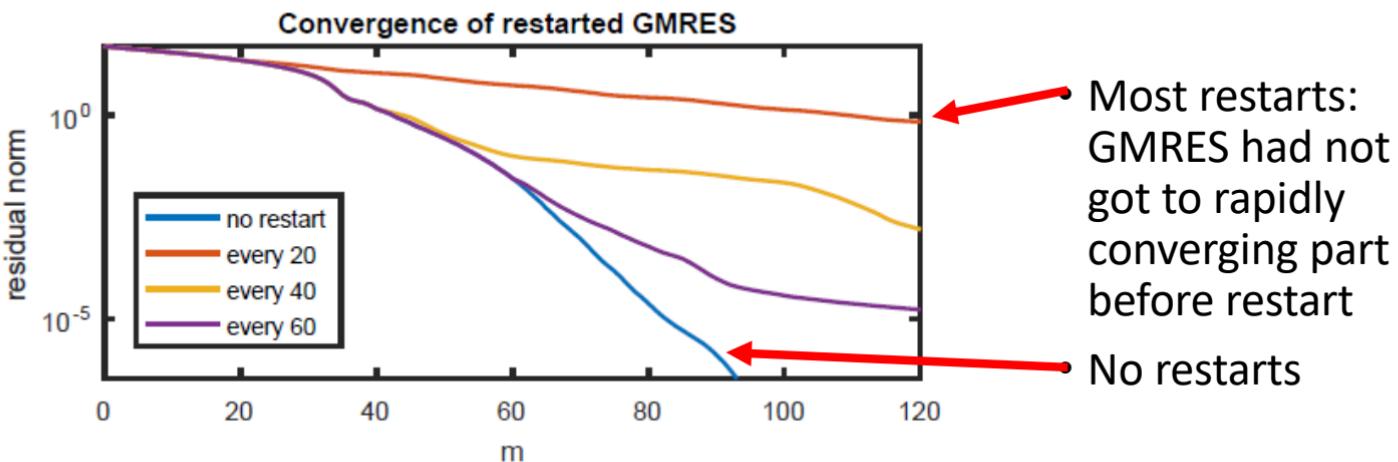
[X, FLAG, RELRES, ITER, RESVEC] = gmres(A, B, ...) also returns a vector of the residual norms at each inner iteration, including NORM(B-A*X0). Note with preconditioners M1,M2, the residual is NORM(M2\ (M1\ (B-A*X))).

- We use only the last of these five outputs here
- X is approximate answer is X
- RELRES gives relative residual of X, $\|B-A^*X\|/\|B\|$
- FLAG states whether we achieved the tolerance
- ITER returns the outer and inner iteration number of the solution
- **RESVEC** is the list of residual values over iterations $\|B-A^*X\|$

Example: GMRES with restarting

Example 8.5.2

```
rest = [maxit 20 40 60];
for j = 1:4
    [~,~,~,~,rv] = gmres(A,b,rest(j),rtol,maxit/rest(j));
    semilogy(0:length(rv)-1,rv,'-'), hold on
end
```



GMRES: comments

- There are a lot of variations for solving $Ax = b$ using Krylov based methods
- These include
 - QMR: quasi-minimal residual
 - CGS: conjugate gradient stabilized
 - BiCGStab: bi-conjugate gradient stabilized
 - And more...
- We will discuss two special cases in the next section

Section 8.6

MINRES and conjugate gradients

Special cases of GMRES

- Some really nice simplifications can be made in special cases of solving $\mathbf{A}\mathbf{x} = \mathbf{b}$, depending on the properties of \mathbf{A}
- Consider Hermitian \mathbf{A} , where $\mathbf{A}^* = \mathbf{A}$
- For square systems, we know that $\mathbf{A}\mathbf{Q}_m = \mathbf{Q}_{m+1}\mathbf{H}_m$
- Use the nice properties of an orthogonal matrix: pre-multiply by \mathbf{Q}_m^* to get

$$\mathbf{Q}_m^* \mathbf{A} \mathbf{Q}_m = \mathbf{Q}_m^* \mathbf{Q}_{m+1} \mathbf{H}_m = \widetilde{\mathbf{H}}_m,$$

- $\widetilde{\mathbf{H}}_m$ is first m rows of \mathbf{H}_m , and it's Hessenberg form
- The lhs is Hermitian; the rhs must be too: $\widetilde{\mathbf{H}}_m$ is tridiagonal!

Special cases of GMRES: MINRES

- This is news we can use!
- The Arnoldi iteration has only a few components at each step:

$$Aq_m = H_{m-1,m} q_{m-1} + H_{mm} q_m + H_{m+1,m} q_{m+1}.$$

- We only need to find $H_{m-1,m}$, H_{mm} , $H_{m+1,m}$, q_{m+1}
- This truncated version of Arnoldi iteration is called *Lanczos iteration*
- Perhaps the best thing about this is that we need only a couple of previous vectors and a few coefficients each step
- This is only $O(1)$ steps per iteration: No need for restarts!

MINRES

- Matlab has a built-in function `minres`
- It also is relatively tractable for convergence analysis.
- If A is hermitian, then it has real eigenvalues
- Let $s_+ = \{\lambda_i | \lambda > 0\}$ and define $\kappa_+ = \max \lambda_i / \min \lambda_i$
- Let $s_- = \{\lambda_i | \lambda < 0\}$ and define $\kappa_- = \min \lambda_i / \max \lambda_i$

$$\frac{\|r_m\|_2}{\|b\|_2} \leq \left(\frac{\sqrt{\kappa_+ \kappa_-} - 1}{\sqrt{\kappa_+ \kappa_-} + 1} \right)^{\lfloor m/2 \rfloor},$$

- $\lfloor m/2 \rfloor$ is the floor function (round $m/2$ down to nearest integer)
- If $\kappa_+ \kappa_-$ is large, the ratio inside the parens tends to unity, and the convergence is slow

MINRES

- Matlab has a built-in function `minres`
- It also is relatively tractable for convergence analysis.
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- Let $s_+ = \{\lambda_i | \lambda > 0\}$ and define $\kappa_+ = \max \lambda_i / \min \lambda_i$
- Let $s_- = \{\lambda_i | \lambda < 0\}$ and define $\kappa_- = \min \lambda_i / \max \lambda_i$

$$\frac{\|r_m\|_2}{\|b\|_2} \leq \left(\frac{\sqrt{\kappa_+ \kappa_-} - 1}{\sqrt{\kappa_+ \kappa_-} + 1} \right)^{\lfloor m/2 \rfloor},$$

- $\lfloor m/2 \rfloor$ is the floor function (round $m/2$ down to nearest integer)
- If $\kappa_+ \kappa_-$ is large, the ratio inside the parens tends to unity, and the convergence is slow

The conjugate gradient method

- Let's specify that nonsingular \mathbf{A} from $\mathbf{Ax} = \mathbf{b}$ is HPD
- Then \mathbf{A} has a Cholesky factorization: $\mathbf{A} = \mathbf{R}^* \mathbf{R}$
- For any vector \mathbf{u} , we have

$$\mathbf{u}^* \mathbf{A} \mathbf{u} = (\mathbf{R}\mathbf{u})^* (\mathbf{R}\mathbf{u}) = \|\mathbf{R}\mathbf{u}\|^2,$$

- This is great because it is non-negative, and zero iff $\mathbf{u} = \mathbf{0}$
- We can then define

$$\|\mathbf{u}\|_{\mathbf{A}} = (\mathbf{u}^* \mathbf{A} \mathbf{u})^{1/2}.$$

- The conjugate gradient method minimizes the error measured with the \mathbf{A} -norm over the sequence of Krylov subspaces
- That is, it computes $\min_{\mathcal{K}_m} \|\mathbf{x}_m - \mathbf{x}\|_{\mathbf{A}}$

The conjugate gradient method

- The conjugate gradient (CG) computes directions for each iterate that are “A-orthogonal” and estimates how long they should be.
- Another take on CG based on this view on the Sakai site
- It began being designed for n steps, i.e., as a direct method, but suffered from the same problem as Krylov iteration.
- Only later did it become a useful iterative method.
- The classical CG method is somewhat limited by the need for an HPD matrix
- But, that same list of modified functions applied to the CG method
- Matlab has a built-in function `pcg`

Convergence of MINRES and CG

- Let A be real and nonsingular with $\kappa = \left\| A^{-1} \right\|_2 \left\| A \right\|_2$
- We have the following theorem:

Theorem 8.6.1

Let A be real and SPD with 2-norm condition number κ . For MINRES define $R(m) = \|r_m\|_2/\|b\|_2$, and for CG define $R(m) = \|x_m - x\|_A/\|x\|_A$, where r_m and x_m are the residual and solution approximation associated with the space \mathcal{K}_m . Then

$$R(m) \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m. \quad (8.6.4)$$

- MINRES: bound on *relative residual*; CG: on *relative error*
- If κ is large, convergence is slow: spectrum of A matters!
- Bigger exponent than indefinite case

Convergence of MINRES and CG

- Using this result, we can estimate how many steps are needed.
- Let κ be a parameter (i.e., given)
- We want to specify a tolerance, say ϵ ; to get the bound under this value, we need

$$2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m \approx \epsilon$$

- Solve for m :

$$m \log \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right) \approx \log \left(\frac{\epsilon}{2} \right).$$

- Simplify assuming large κ :

$$\begin{aligned} \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} &= (1 - \kappa^{-1/2})(1 + \kappa^{-1/2})^{-1} \\ &= (1 - \kappa^{-1/2})(1 - \kappa^{-1/2} + \kappa^{-1} + \dots) \\ &= 1 - 2\kappa^{-1/2} + O(\kappa^{-1}), \quad \text{as } \kappa \rightarrow \infty. \end{aligned}$$

Convergence of MINRES and CG

- Now use the last result inside the log function and Taylor expand to get

$$\log(1 + x) = x - (x^2/2) + \dots,$$

- Finally, we obtain

$$-2m\kappa^{-1/2} \approx \log\left(\frac{\epsilon}{2}\right), \text{ or } m = O(\sqrt{\kappa}),$$

- It is easy to see that the number of iterations m increases with $\kappa^{1/2}$ and with decreasing tolerance ϵ
- Let's do an example

Example: MINRES and CG

Example 8.6.1

```
n = 1000;
density = 0.008;
A = sprandsym(n,density,1e-2,2);
x = (1:n)'/n;
b = A*x;
```

- Create sparse random matrix
- Condition number 100
- Known solution

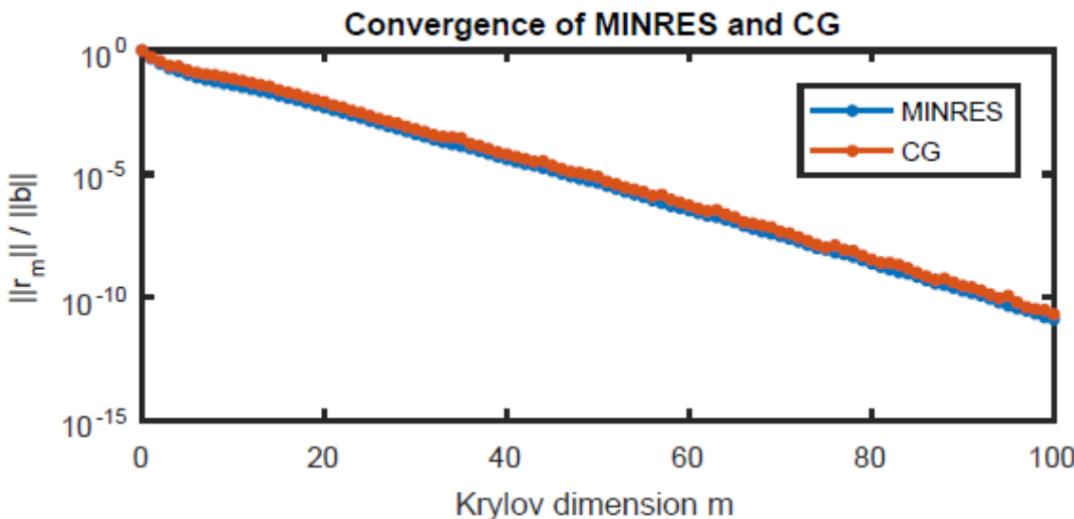
```
[xMR,~,~,~,residMR] = minres(A,b,1e-12,100);
[xCG,~,~,~,residCG] = pcg(A,b,1e-12,100);
semilogy(0:100,residMR/norm(b),'.-')
hold on, semilogy(0:100,residCG/norm(b),'.-')
```

- `minres` used first
- `pcg` second
- Same tolerance
- Plot relative residuals

Example: MINRES and CG

Example 8.6.1

```
[xMR,~,~,~,residMR] = minres(A,b,1e-12,100);  
[xCG,~,~,~,residCG] = pcg(A,b,1e-12,100);  
semilogy(0:100,residMR/norm(b),'.-')  
hold on, semilogy(0:100,residCG/norm(b),'.-')
```



- `minres` and `pcg` residuals are very similar here
- What about error?
- We know exact solution here

Example: MINRES and CG

Example 8.6.1

```
errorMR = norm( xMR - x ) / norm(x)
errorCG = norm( xCG - x ) / norm(x)
```

```
errorMR =
    1.1192e-10
errorCG =
    7.9932e-11
```

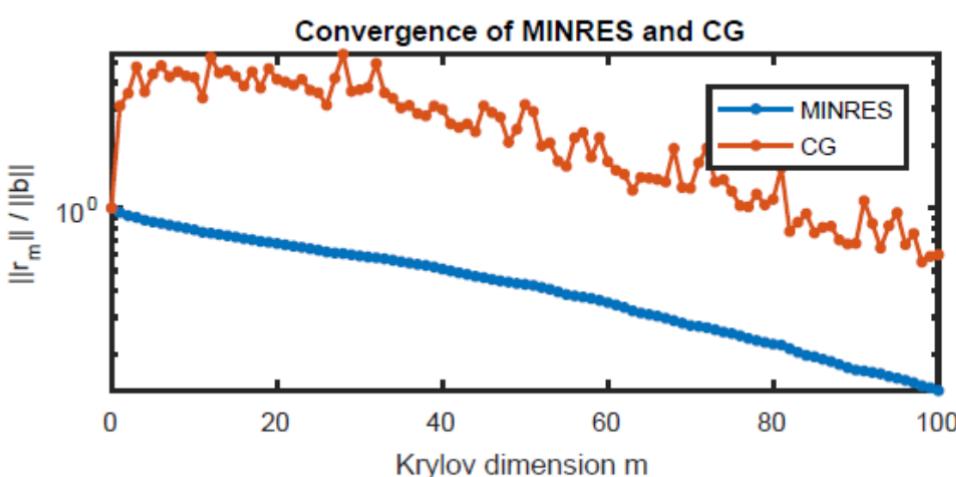
```
A = sprandsym(n,density,1e-4,2);
```

- Using the exact solution, we see little difference when the condition number is $\kappa = 100$
- Now let's up the ante and use a condition number of $\kappa = 10^4$

Example: MINRES and CG

Example 8.6.1

```
[xMR ,~,~,~,residMR] = minres(A,b,1e-12,100);  
[xCG ,~,~,~,residCG] = pcg(A,b,1e-12,100);  
clf  
semilogy(0:100,residMR/norm(b),'.-')  
hold on, semilogy(0:100,residCG/norm(b),'.-')
```



- `minres` and `pcg` residuals' decay *rates* are similar, but residual bigger for CG
- Very little progress toward answer
- What about error?

Example: MINRES and CG

Example 8.6.1

```
errorMR = norm( xMR - x ) / norm(x)
errorCG = norm( xCG - x ) / norm(x)
```

```
errorMR =
  922.3604
errorCG =
  1.0061e+03
```

- Yep, that error is bad!
- Theory: $\kappa = 100, 2 \left(\frac{9}{11} \right)^{100} \approx 3.9 \times 10^{-9}$
- Theory: $\kappa = 10^4, 2 \left(\frac{99}{101} \right)^{100} \approx 0.27$
- Larger κ has strong effect!

$$R(m) \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m$$

About stopping criteria

- $\mathbf{A}\mathbf{x} = \mathbf{b}$; in m th iteration is \mathbf{x}_m ; $\mathbf{r}_m = \mathbf{b} - \mathbf{A}\mathbf{x}_m$
- We can think of solution as $\mathbf{x} = \mathbf{x}_m + \boldsymbol{\delta}_m$
- Substitution gives $\mathbf{A}(\mathbf{x}_m + \boldsymbol{\delta}_m) = \mathbf{b}$, or $\mathbf{A}\boldsymbol{\delta}_m = \mathbf{b} - \mathbf{A}\mathbf{x}_m = \mathbf{r}_m$
- Approximately solving $\mathbf{A}\boldsymbol{\delta}_m = \mathbf{r}_m$ for the “correction” gives us an updated solution $\mathbf{x}_{m+1} = \mathbf{x}_m + \boldsymbol{\delta}_m$
- Iteration can be stopped when $\|\boldsymbol{\delta}_m\|$ or $\|\mathbf{r}_m\|$, or both, are smaller than preset tolerances
- When \mathbf{A} is ill-conditioned, $\|\mathbf{r}_m\|$ may be very small, while $\|\boldsymbol{\delta}_m\|$ isn't: be careful

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \kappa(A) \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}. \quad (2.8.4)$$

Section 8.7

Matrix-free Iterations

Linear transformations, and undoing them

- We can think of $\mathbf{A}\mathbf{x} = \mathbf{b}$ as a linear transformation of \mathbf{x} to \mathbf{b}
- The solution process undoes this transformation,
$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$
- Interestingly, we can undo a linear transformation without having to explicitly form the matrix \mathbf{A}^{-1} !
- How can we do this? Let's try an example.

Linear transformations, and undoing them

- We can think of $\mathbf{A}\mathbf{x} = \mathbf{b}$ as a linear transformation of \mathbf{x} to \mathbf{b}
- The solution process undoes this transformation,
$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$
- Interestingly, we can undo a linear transformation without having to explicitly form the matrix \mathbf{A}^{-1} !
- How can we do this? Let's try an example.

Blurring images

- We can think of an image as an $m \times n$ matrix \mathbf{X} , as we've already done
- Let's consider a simple model process for blurring
- Let the tridiagonal $m \times n$ matrix \mathbf{B} be given by

$$B_{ij} = \begin{cases} \frac{1}{2}, & \text{if } i = j \\ \frac{1}{4}, & \text{if } |i - j| = 1 \\ 0, & \text{otherwise.} \end{cases}$$

- Pre-multiplication forms weighted combos or averages of elements in each column: \mathbf{BX}
- This smears column elements

Blurring images

- For rows, we can make a matrix with elements as it B , but make it $n \times n$
- Call this tridiagonal matrix C
- We can accomplish row blurring with transposes

$$(\textcolor{brown}{C} \textcolor{blue}{X}^T)^T = \textcolor{blue}{X} \textcolor{brown}{C}^T = \textcolor{blue}{X} \textcolor{brown}{C}$$

- We can get blurring of both rows and columns with

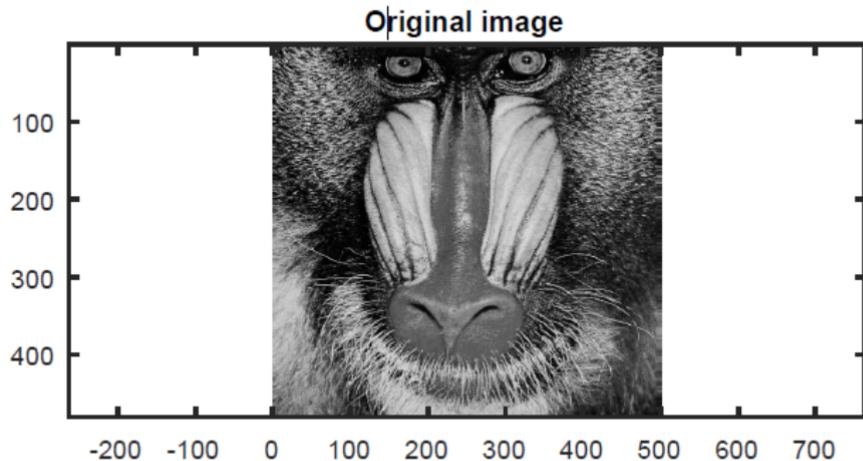
$$\text{blur}(\textcolor{blue}{X}) = \textcolor{brown}{B}^k \textcolor{blue}{X} \textcolor{brown}{C}^k$$

- Integer $k \geq 1$

Blurring example

Example 8.7.1

```
load mandrill  
[m,n] = size(X)  
image(X), colormap(gray(256))  
  
m =  
    480  
n =  
    500
```



- We use our best old ex-friend the mandrill
- Now make some blurring matrices, and combine them for a blur function

```
v = [1/4 1/2 1/4];  
B = spdiags( repmat(v,m,1), -1:1, m,m);  
C = spdiags( repmat(v,n,1), -1:1, n,n);  
  
blur = @(X) B^12 * X * C^12;
```

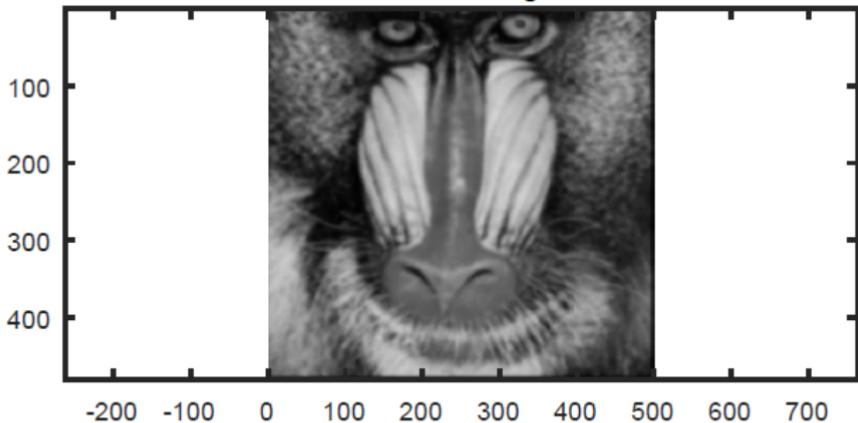
Blurring example

Example 8.7.1

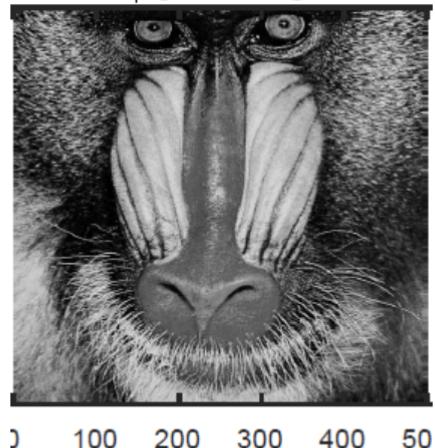
This is what the blur did at left

```
image(blur(X))
```

Blurred image



Original image



Deblurring images

- An important task is to try to deblur poorly focused images
- One way to treat this process is as linear transformation of the image
- To facilitate this, convert the $m \times n$ matrix \mathbf{X} to an $mn \times 1$ vector \mathbf{x}
- Denote this by $\text{vec}(\mathbf{X}) = \mathbf{x}$
- Converting from vector to matrix will be $\text{unvec}(\mathbf{x}) = \mathbf{X}$
- We use blurring process from before $\mathbf{Z} = \text{blur}(\mathbf{X})$

Deblurring images

- Because the blurring is a linear transformation, we can write it as $\mathbf{A} \text{vec}(\mathbf{X}) = \text{vec}(\mathbf{Z})$.
- The matrix \mathbf{A} is $mn \times mn$
- For a 12 megapixel image, 1.4×10^4 entries!!!
- The matrix is very sparse but it is not necessary
- Given an input vector \mathbf{u} , we can compute $\mathbf{v} = \mathbf{A}\mathbf{u}$ via

$$\mathbf{U} = \text{unvec}(\mathbf{u})$$

$$\mathbf{V} = \text{blur}(\mathbf{U})$$

$$\mathbf{v} = \text{vec}(\mathbf{V}).$$

- Our blur recipe can be used without constructing \mathbf{A}

Deblurring example

Example 8.7.2

```
load mandrill
[m,n] = size(X)
v = [1/4 1/2 1/4];
B = spdiags( repmat(v,m,1), -1:1, m,m);
C = spdiags( repmat(v,n,1), -1:1, n,n);
blur = @(X) B^12 * X * C^12;
Z = blur(X);

m =
    480
n =
    500

vec = @(X) reshape(X,m*n,1);
unvec = @(x) reshape(x,m,n);
T = @(x) vec(blur(unvec(x)));
```

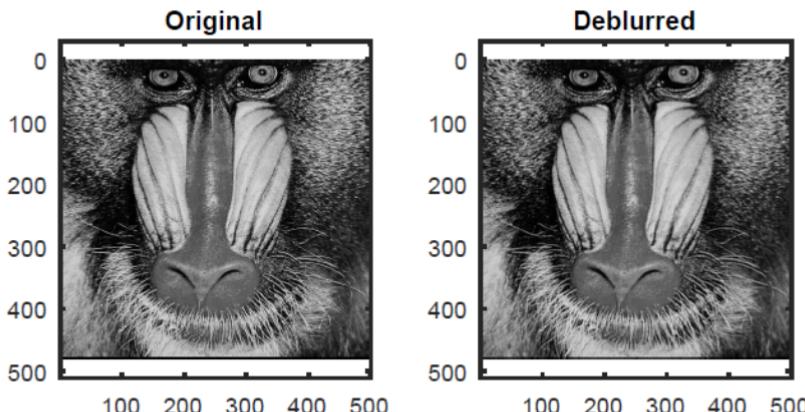
- Mandrill again
- Imagine blurred image Z is given and we want to get back unblurred version X
- Make vec, unvec and blur
- T defines the action of the matrix A but does not create it

Deblurring example

Example 8.7.2

```
y = gmres(T, vec(Z), 50, 1e-5);  
Y = unvec(y);  
subplot(121)  
image(X), colormap(gray(256))  
subplot(122)  
image(Y), colormap(gray(256))
```

```
gmres(50) converged at outer iteration 2 (inner iteration  
45) to a solution with relative residual 1e-05.
```



- Apply GMRES to finding the inverse of the blur transformation
- The function T is passed in rather than the matrix: this effectively says how to compute the matrix vector produce Au
- Not a perfect deblurring

Section 8.8

Preconditioning

Preconditioning

- As condition number increases, convergence of Krylov methods deteriorates
- Preconditioning can help get around this
- Say we are solving $\mathbf{A}\mathbf{x} = \mathbf{b}$
- The idea is to use an easily inverted matrix that is close the original \mathbf{A} that gives a better conditioned system
- Say we are choosing \mathbf{M}
- Then we are trying to find it so that $(\mathbf{M}^{-1}\mathbf{A})\mathbf{x} = (\mathbf{M}^{-1}\mathbf{b})$ is easier to solve
- Do we compute \mathbf{M}^{-1} ? NO!!!!!!

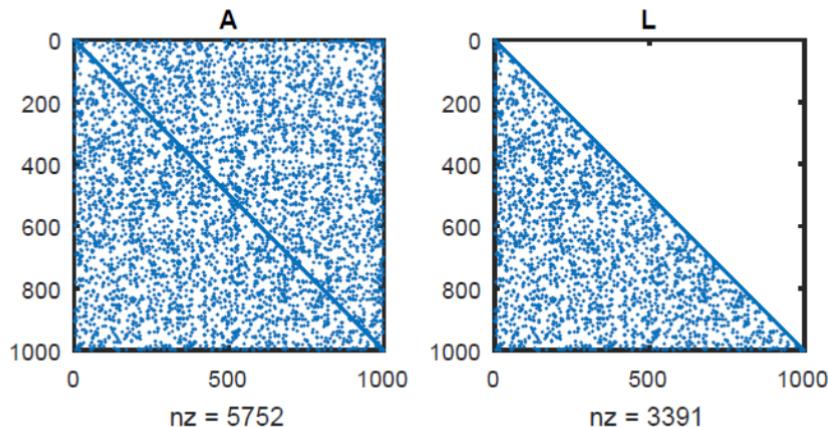
Preconditioning

- We want \mathbf{M} so that $(\mathbf{M}^{-1}\mathbf{A})\mathbf{x} = (\mathbf{M}^{-1}\mathbf{b})$ is easier to solve
- Instead of \mathbf{M}^{-1} , we do the following two step process to compute any $\mathbf{y} = (\mathbf{M}^{-1}\mathbf{A})\mathbf{v}$
 1. Set $\mathbf{u} = \mathbf{A}\mathbf{v}$.
 2. Solve $\mathbf{M}\mathbf{y} = \mathbf{u}$ for \mathbf{y} .
- We use a numerical solve which is more efficient than inverting a matrix
- How to get \mathbf{M} ? One approach is *incomplete LU factorization*, or ILU factorization

Preconditioning: ILU

- We know that LU factorization can ruin sparsity
- ILU says to only save nonzero elements that are similar to the original matrix
- Alternatively, one can set threshold and set to zero any element smaller than that

```
[L,U] = ilu(A);  
subplot(121), spy(A)  
subplot(122), spy(L)
```

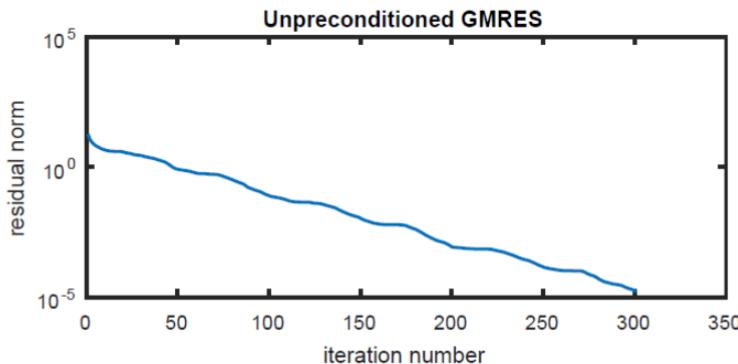


Preconditioning example

Example 8.8.1

Here is a 1000×1000 matrix of density around 0.5%.

```
A = 0.6*speye(1000) + sprand(1000,1000,0.005,1/10000);  
b = rand(1000,1);  
[x,~,~,~,resid_plain] = gmres(A,b,50,1e-10,6); % restart  
at 50  
clf, semilogy(resid_plain,'-')
```

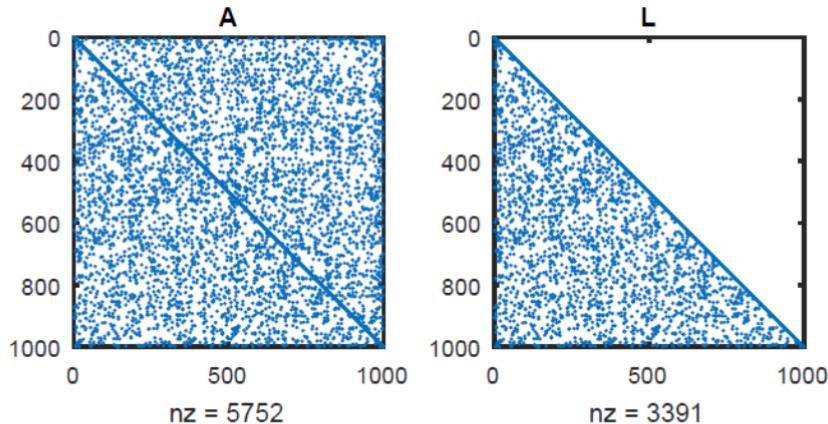


- Slow convergence for this system

Preconditioning example

Example 8.8.1

```
[L,U] = ilu(A);
subplot(121), spy(A)
subplot(122), spy(L)
```



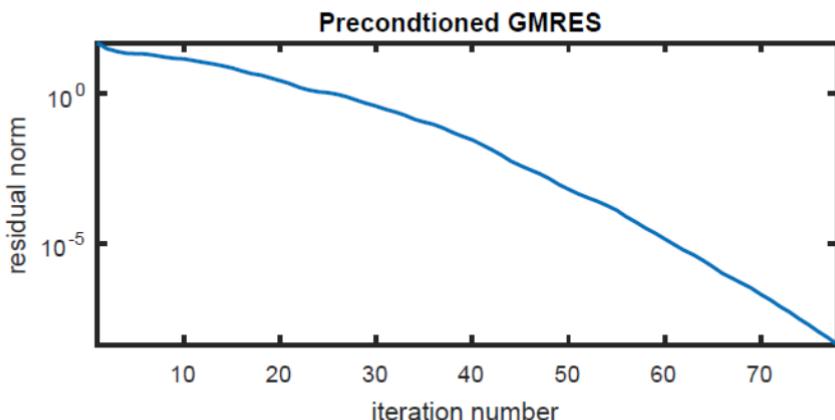
It does *not* produce a true factorization of A .

```
norm( full(A - L*U) )
```

Preconditioning example

Example 8.8.1

```
[x,~,~,~,resid_prec] = gmres(A,b,[],1e-10,300,L,U);  
clf, semilogy(resid_prec,'-')
```



- Better now

Preconditioning

- We want \mathbf{M} so that $(\mathbf{M}^{-1}\mathbf{A})\mathbf{x} = (\mathbf{M}^{-1}\mathbf{b})$ is easier to solve
- Not always easy to find
- Our last example found $\mathbf{M} = \mathbf{L}\mathbf{U}$
- If we were doing this manually we would need to solve $(\mathbf{M}^{-1}\mathbf{b}) = \mathbf{c}$, or $\mathbf{c} = \mathbf{U}\backslash(\mathbf{L}\backslash\mathbf{b})$ to get the rhs
- Then use our previous two-step procedure to solve the preconditioned system
 1. Set $\mathbf{u} = \mathbf{A}\mathbf{v}$.
 2. Solve $\mathbf{M}\mathbf{y} = \mathbf{u}$ for \mathbf{y} .